

2,2,2-Trifluoroethanol
75-89-8 | DTXSID0021751

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -35.9 °C

Global applicability domain: Inside

Local applicability domain index: 5.19e-01

Confidence level: 5.74e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,2,2-Trifluoroethanol</div> <div>Measured: -43.5</div> <div>Predicted: -35.9</div>	<div>Image not found</div> <div>1-Propanol, 2,2,3,3-tetrafluoro-</div> <div>Measured: -15.0</div> <div>Predicted: -15.0</div>	<div>Image not found</div> <div>Difluoroethanol</div> <div>Measured: -28.2</div> <div>Predicted: -15.9</div>
<div>Image not found</div> <div>Acetic acid, trifluoro-</div> <div>Measured: -15.2</div> <div>Predicted: -15.5</div>	<div>Image not found</div> <div>Acetic acid, difluoro-</div> <div>Measured: -1.00</div> <div>Predicted: 19.4</div>	